201-15756

IUCLID

Data Set

Existing Chemical	:	ID: 68609-68-7
CAS No.	:	68609-68-7
Producer related part		
Company	:	BASF Corporation
Creation date	:	30.12.2003
Substance related part		
Company	:	BASF Corporation
Creation date	:	30.12.2003
Status	:	
Memo	:	Prepared by: Toxicology and Regulatory Affairs Freeburg IL 62243 618-538-5280
Printing date	:	24.12.2004
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Chapter (profile)	:	Chapter: 1.0.1, 1.2, 2.1, 2.2, 2.3, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.3.2, 3.5, 4.1, 4.2, 4.3, 4.4, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.7, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.2 SYNONYMS AND TRADENAMES

2.1 MELTING POINT

Value : ca. -62 °C

Remark :
As this material is a variable mixture this must be considered as only an approximation of the actual freezing point for any batch.

Test substance :
EP-204 CASNO 68609-68-7

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
30.12.2003 (6)

2.2 BOILING POINT

Value : ca. 180 - 350 °C at 1013 hPa

Remark :
As this material is a variable mixture this must be considered as only an approximation of the boiling point for any batch.

Test substance :
EP-204 CASNO 68609-68-7

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
02.01.2004 (1)

2.4 VAPOUR PRESSURE

Value : ca. 1 - 5 hPa at 25 °C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance :

Method :
The vapor pressure for the mixture is estimated using the mean of the Antoine & Grain methods as calculated using the MPBPWIN v1.40 program found in EPIWIN 3.05. The initial boiling point and the final boiling point are the only input parameters this estimate is based on, as the program is insensitive to structure if a determined boiling point is an input. Likewise, the program is insensitive to melting point when calculating VPs for liquids.

The structure for 2-ethylhexyl-1,3-diol was entered to provide a reference value for one of the pure components.

As this is a variable mixture, the initial and final boiling point values are also variable

Result :

Experimental Database Structure Match:
Name : 2-ETHYL-1,3-HEXANDIOL
CAS Num : 000094-96-2
Exp MP (deg C): -40
Exp BP (deg C): 244
Exp VP (mm Hg): 3.00E-03 (extrapolated)
Exp VP (deg C): 25
Exp VP ref : BLAINE,RL (1976)

SMILES : CCCC(O)C(CC)CO
CHEM : EP-204
MOL FOR: C8 H18 O2
MOL WT : 146.23

+++++++BASED ON INITIAL BP OF 180 deg C

---------- SUMMARY MPBPWIN v1.40 ----------

Boiling Point: 242.50 deg C (Adapted Stein and Brown Method)

Melting Point: -1.60 deg C (Adapted Joback Method)
Melting Point: 27.93 deg C (Gold and Ogle Method)
Mean Melt Pt : 13.17 deg C (Joback; Gold,Ogle Methods)
Selected MP: 13.17 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 180.00 deg C (user entered))
(MP not used for liquids)
VP: 0.197 mm Hg (Antoine Method)
VP: 0.157 mm Hg (Modified Grain Method)
VP: 1.37 mm Hg (Mackay Method)
Selected VP: 0.177 mm Hg (Mean of Antoine & Grain methods)

+++++++++ BASED ON FINAL BP OF 350 dec C
---------- SUMMARY MPBPWIN v1.40 ----------
Boiling Point: 242.50 deg C (Adapted Stein and Brown Method)
Melting Point: -1.60 deg C (Adapted Joback Method)
Melting Point: 27.93 deg C (Gold and Ogle Method)
Mean Melt Pt : 13.17 deg C (Joback; Gold,Ogle Methods)
Selected MP: 13.17 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 350.00 deg C (user entered))
(MP not used for liquids)
VP: 9.62E-007 mm Hg (Antoine Method)
VP: 2.5E-006 mm Hg (Modified Grain Method)
VP: 0.000262 mm Hg (Mackay Method)
Selected VP: 2.5E-006 mm Hg (Modified Grain Method)

Test substance :

EP-204 CASNO 68609-68-7

Conclusion

The calculated vapor pressure for this mixture, assuming it is a pure material of boiling point 180 deg C, is approximately 0.2 mm Hg. As this is a variable mixture, a specific VP cannot be stated. It is concluded that giving the VP as a range of 0.1 to 2 hPa is a conservative yet realistic estimate.

Reliability : (2) valid with restrictions

Estimates using an acceptable method are assigned a reliability score of 2.

Flag : Critical study for SIDS endpoint

02.01.2004 (15) (18)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : at °C
pH value :
Method :
Year :
GLP :
Test substance : other TS

Method :

Octanol water partition coefficients for the major components of EP-202 were obtained through the KOWWIN program (v1.66) by entering the structure of the component into the program using the SMILES code. These codes are listed in the results section. Where there was an experimental value found in the database associated with the program, that value was accepted. Where an experimental value was not found the program estimate was accepted.

Result :

KOWWIN Program (v1.66) Results:

SMILES : CCCCC(CC)CO
CHEM : 2-Ethylhexanol
MOL FOR: C8 H18 O1
MOL WT : 130.23
Log Kow(version 1.66 estimate): 2.73

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	5	-CH2- [aliphatic carbon]	0.4911	2.4555
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	-OH [hydroxy, aliphatic attach]	-1.4086	-1.4086
Const		Equation Constant		0.2290
			Log Kow =	2.7319

SMILES : CCCC=C(CC)C=O
CHEM : 2-Ethylhexenal
MOL FOR: C8 H14 O1
MOL WT : 126.20
Log Kow(version 1.66 estimate): 2.62

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	3	-CH2- [aliphatic carbon]	0.4911	1.4733
Frag	2	=CH- or =C< [olefinc carbon]	0.3836	0.7672
Frag	1	-CHO [aldehyde, aliphatic attach]	-0.9422	-0.9422
Const		Equation Constant		0.2290
			Log Kow =	2.6219

SMILES : CCCCC(CC)C=O
CHEM : 2-Ethylhexanal
MOL FOR: C8 H16 O1
MOL WT : 128.22
Log Kow(version 1.66 estimate): 2.71

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	4	-CH2- [aliphatic carbon]	0.4911	1.9644
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	-CHO [aldehyde, aliphatic attach]	-0.9422	-0.9422
Const		Equation Constant		0.2290
			Log Kow =	2.7072

SMILES : CCCCO
CHEM : n-Butanol
MOL FOR: C4 H10 O1
MOL WT : 74.12
Log Kow(version 1.66 estimate): 0.84
Experimental Database Structure Match:
Name : 1-Butanol
CAS Num : 000071-36-3
Exp Log P: 0.88
Exp Ref : Hansch,C et al. (1995)

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	3	-CH2- [aliphatic carbon]	0.4911	1.4733
Frag	1	-OH [hydroxy, aliphatic attach]	-1.4086	-1.4086
Const		Equation Constant		0.2290
			Log Kow =	0.8410

SMILES : CCCC(O)C(CC)CO
CHEM : 2-Ethyl-1,3-hexanediol
MOL FOR: C8 H18 O2
MOL WT : 146.23
Log Kow(version 1.66 estimate): 1.60

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	4	-CH2- [aliphatic carbon]	0.4911	1.9644
Frag	2	-CH [aliphatic carbon]	0.3614	0.7228
Frag	2	-OH [hydroxy, aliphatic attach]	-1.4086	-2.8172
Factor	1	Multi-alcohol correction	0.4064	0.4064
Const		Equation Constant		0.2290
			Log Kow =	1.6000

SMILES : CCCC(OC(=O)CCC)C(CC)COC(=O)CCC
CHEM : 2-Ethylhexyl-1,3-dibutyrate
MOL FOR: C16 H30 O4
MOL WT : 286.42
Log Kow(version 1.66 estimate): 5.17

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	4	-CH3 [aliphatic carbon]	0.5473	2.1892
Frag	8	-CH2- [aliphatic carbon]	0.4911	3.9288
Frag	2	-CH [aliphatic carbon]	0.3614	0.7228
Frag	2	-C(=O)O [ester, aliphatic attach]	-0.9505	-1.9010
Const		Equation Constant		0.2290
			Log Kow =	5.1688

SMILES : CCCC(=O)OCCCC
CHEM : N-butyl-n-butyrate
MOL FOR: C8 H16 O2
MOL WT : 144.22
Log Kow(version 1.66 estimate): 2.83

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	5	-CH2- [aliphatic carbon]	0.4911	2.4555
Frag	1	-C(=O)O [ester, aliphatic attach]	-0.9505	-0.9505
Const		Equation Constant		0.2290
			Log Kow =	2.8286

SMILES : CCCC=O
CHEM : N-butyraldehyde
MOL FOR: C4 H8 O1
MOL WT : 72.11
Log Kow(version 1.66 estimate): 0.82

Experimental Database Structure Match:
Name : Butyraldehyde
CAS Num : 000123-72-8
Exp Log P: 0.88
Exp Ref : Hansch,C et al. (1995)

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	2	-CH2- [aliphatic carbon]	0.4911	0.9822
Frag	1	-CHO [aldehyde, aliphatic attach]	-0.9422	-0.9422
Const		Equation Constant		0.2290
			Log Kow =	0.8163

SMILES : CCCCC(CC)CC(CC)CO
CHEM : 2,4-Diethyloctane-1-ol
MOL FOR: C12 H26 O1
MOL WT : 186.34

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH3 [aliphatic carbon]	0.5473	1.6419
Frag	7	-CH2- [aliphatic carbon]	0.4911	3.4377
Frag	2	-CH [aliphatic carbon]	0.3614	0.7228
Frag	1	-OH [hydroxy, aliphatic attach]	-1.4086	-1.4086
Const		Equation Constant		0.2290
			Log Kow =	4.6228

SMILES : CCCC(O)C(CC)CC(CC)CO
CHEM : 2,4-Diethyloctane-1,5-diol
MOL FOR: C12 H26 O2
MOL WT : 202.34

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH3 [aliphatic carbon]	0.5473	1.6419
Frag	6	-CH2- [aliphatic carbon]	0.4911	2.9466
Frag	3	-CH [aliphatic carbon]	0.3614	1.0842
Frag	2	-OH [hydroxy, aliphatic attach]	-1.4086	-2.8172
Factor	1	Multi-alcohol correction	0.4064	0.4064
Const		Equation Constant		0.2290
			Log Kow =	3.4909

SMILES : CCC(CO)C(CCC)C(CO)CC
CHEM : 2-Ethyl-3-propyl-4-hydroxymethylhexan-1-ol (C12-diol)
MOL FOR: C12 H26 O2
MOL WT : 202.34

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH3 [aliphatic carbon]	0.5473	1.6419
Frag	6	-CH2- [aliphatic carbon]	0.4911	2.9466
Frag	3	-CH [aliphatic carbon]	0.3614	1.0842
Frag	2	-OH [hydroxy, aliphatic attach]	-1.4086	-2.8172
Factor	1	Multi-alcohol correction	0.4064	0.4064
Const		Equation Constant		0.2290
			Log Kow =	3.4909

SMILES : CCC(CO)CC(CC)C(CCC)C(CO)CC
CHEM : 2,4,6-Triethyl-3-propylheptane-1,7-diol (C16-diol)
MOL FOR: C16 H34 O2
MOL WT : 258.45

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	4	-CH3 [aliphatic carbon]	0.5473	2.1892
Frag	8	-CH2- [aliphatic carbon]	0.4911	3.9288
Frag	4	-CH [aliphatic carbon]	0.3614	1.4456
Frag	2	-OH [hydroxy, aliphatic attach]	-1.4086	-2.8172
Factor	1	Multi-alcohol correction	0.4064	0.4064
Const		Equation Constant		0.2290
			Log Kow =	5.3818

SMILES : CCCCC(CC)COCCCC
CHEM : 2-Ethylhexyl-n-butyl ether
MOL FOR: C12 H26 O1
MOL WT : 186.34

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH3 [aliphatic carbon]	0.5473	1.6419
Frag	8	-CH2- [aliphatic carbon]	0.4911	3.9288
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	1	-O- [oxygen, aliphatic attach]	-1.2566	-1.2566
Const		Equation Constant		0.2290
			Log Kow =	4.9045

Test substance :

Various individal componets of EP-204, CASNO 68609-68-7

Conclusion :

The following values were found for log Kow

COMPONENT********	**log Kow**
2-Ethylhexanol	2.73 c
2-Ethylhexenal	2.62 c
2-Ethylhexanal	2.71 c
N-butanol	0.88 e
2-Ethyl-1,3-hexanediol	1.60 c
2-Ethylhexyl-1,3-dibutyrate	5.17 c
2,4-Diethyloctane-1-ol	4.62 c
2,4-Diethyloctane-1,5-diol	3.49 c
2-Ethyl-3-propyl-4-hydroxymethylhexan-1-ol	3.49 c
2,4,6-Triethyl-3-propylheptane-1,7-diol	4.89 c
N-butyl-n-butyrate	2.83 c
N-butyraldehyde	-0.48 e

e = experimental
c = calculated

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
24.12.2004 (20)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : at °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

Method :

Water solubility estimates and experimental values for the major components of EP-202 were obtained through the WSKOW program (v1.40) by entering the structure of the component into the program using the SMILES code. These codes are listed in the results section. Where there was an experimental value found in the database associated with the program, that value was accepted. Where an experimental value was not found the program estimate was accepted.

The following formula was used by the program to estimate the water solubility:

Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction

The only Correction Value that was applied was for the non-diol aliphatic alcohols.

Alcohol, aliphatic 0.510

Result :

The following results were obtained for water solubility:

COMPONENT	***SMILES****	***Kow***	Water Sol **(mg/L)**
2-Ethylhexanol	CCCCC(CC)CO	2.73c	880e
2-Ethylhexenal	CCCC=C(CC)C=O	2.62c	548e
2-Ethylhexanal	CCCCC(CC)C=O	2.71c	400e
n-Butanol	CCCCO	0.88e	63200e
2-Ethyl-1,3-hexanediol	CCCC(O)C(CC)CO	1.60c	4200e
2-Ethylhexyl-1,3-dibutyrate	CCCC(OC(=O)CCC)C(CC)COC(=O)CCC	5.17c	0.57e
n-Butyl-n-butyrate	CCCC(=O)OCCCC	2.83c	309c
n-Butyraldehyde	CCCC=O	-0.48e	2385e
2,4-Diethyloctane-1-ol	CCCCC(CC)CC(CC)CO	4.62c	18.7c
2,4-Diethyloctane-1,5-diol	CCCC(O)C(CC)CC(CC)CO	3.49c	44.4c
2-Ethyl-3-propyl-4-hydroxymethylhexan-1-ol (C12-diol)	CCC(CO)C(CCC)C(CO)CC	3.49c	44.4c
2,4,6-Triethyl-3-propylheptane-1,7-diol (C16-diol)	CCC(CO)CC(CC)C(CCC)C(CO)CC	4.89c	1.69c
2-Ethylhexyl-butyl ether	CCCCC(CC)COCCCC	4.90c	3.32c

e = experimental
c = calculated

Test substance :

Various individal componets of EP-204, CASNO 68609-68-7

Conclusion :

Water solubility varies for components of EP-204 from less than 1 mg/L to greater than 1000 mg/L

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
24.12.2004 (20)

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight

Method :

The structure of the various identified and anticipated components was initially examined to determine if there was a chromophore that could absorb light energy at wavelengths above 295 um. As none of the conjugated systems was likely to absorb light in the appropriate wavelength and as the material is basically colorless, it was assumed that direct photolysis would be unimportant to the fate of the test material.

To estimate indirect photolysis, the various major components were examined using the APOWIN (1.90) program found in EPIWIN. This program estimates the reaction rate of the molecule with hydroxyl radical based on its structural components that are reactive with atmospheric hydroxyl radical. An overall rate constant is estimated and a search is conducted for materials with experimentally determined rate constants. The program then calculates an approximate atmospheric half-life using a (used defined) 12-hour day and hydroxyl radical concentration.

Olefinic compounds were also evaluated for reactivity with atmospheric ozone. Some components were judged to be ozone reactive but the contribution of this sensitizer was negligible as compared to hydroxyl radical and was ignored in constructing the table.

This analysis was conducted for each of the identified major components and structures representative of the various classes of components. Under environmental conditions of essentially infinite dilution, each component is considered to photodegrade independently of the other components in the mixture.

Result :

AOP Program (v1.90) Results:
==========
SMILES : CCCC=C(CC)C=O
CHEM : 2-Ethylhexenal
MOL FOR: C8 H14 O1
MOL WT : 126.20

---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 20.4442 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 29.5460 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 49.9902 E-12 cm3/molecule-sec
HALF-LIFE = 0.214 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 2.568 Hrs

---------- SUMMARY (AOP v1.90): OZONE REACTION ----
OVERALL OZONE Rate Constant = 1.183000 E-17 cm3/molecule-sec
HALF-LIFE = 0.969 Days (at 7E11 mol/cm3)
HALF-LIFE = 23.249 Hrs

Experimental Database: NO Structure Matches

AOP Program (v1.90) Results:
==========
SMILES : CCCCC(CC)C=O
CHEM : 2-Ethylhexanal
MOL FOR: C8 H16 O1
MOL WT : 128.22
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 33.9806 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 33.9806 E-12 cm3/molecule-sec
HALF-LIFE = 0.315 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 3.777 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

AOP Program (v1.90) Results:
==========
SMILES : CCCCO
CHEM : n-Butanol
MOL FOR: C4 H10 O1
MOL WT : 74.12
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 6.7500 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 6.8900 E-12 cm3/molecule-sec
HALF-LIFE = 1.552 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 18.629 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******

(ONLY Olefins and Acetylenes are Estimated)

Experimental Database Structure Match:
Chem Name : 1-Butanol
CAS Number: 000071-36-3
Exper OH rate constant : 8.57 E-12 cm3/molecule-sec
Exper OH Reference: KWOK,ESC & ATKINSON,R (1994)
Exper Ozone rate constant: --- cm3/molecule-sec
Exper NO3 rate constant : --- cm3/molecule-sec

SMILES : CCCC(O)C(CC)CO
CHEM : 2-Ethyl-1,3-hexanediol
MOL FOR: C8 H18 O2
MOL WT : 146.23
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 21.9488 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 22.2288 E-12 cm3/molecule-sec
HALF-LIFE = 0.481 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 5.774 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

==========
SMILES : CCCC(OC(=O)CCC)C(CC)COC(=O)CCC
CHEM : 2-Ethylhexyl-1,3-dibutyrate
MOL FOR: C16 H30 O4
MOL WT : 286.42
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 17.5340 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 17.5340 E-12 cm3/molecule-sec
HALF-LIFE = 0.610 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 7.320 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

SMILES : CCCC(=O)OCCCC
CHEM : n-butyl-n-butyrate
MOL FOR: C8 H16 O2
MOL WT : 144.22
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 6.2395 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 6.2395 E-12 cm3/molecule-sec
HALF-LIFE = 1.714 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 20.571 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database Structure Match:
Chem Name : n-Butyl butyrate
CAS Number: 000109-21-7
Exper OH rate constant : 10.6 E-12 cm3/molecule-sec
Exper OH Reference: ATKINSON,R (1989)
Exper Ozone rate constant: --- cm3/molecule-sec
Exper NO3 rate constant : --- cm3/molecule-sec

HALF-life Based on Experimental Rate Constant: 12.1 hours

==========
SMILES : CCCC=O
CHEM : n-butyraldehyde
MOL FOR: C4 H8 O1
MOL WT : 72.11
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 25.4314 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 25.4314 E-12 cm3/molecule-sec
HALF-LIFE = 0.421 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 5.047 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database Structure Match:
Chem Name : Butanal
CAS Number: 000123-72-8
Exper OH rate constant : 23.5 E-12 cm3/molecule-sec

Exper OH Reference: ATKINSON,R (1985)
Exper Ozone rate constant: --- cm3/molecule-sec
Exper NO3 rate constant : --- cm3/molecule-sec

AOP Program (v1.90) Results:
==========
SMILES : CCCCC(CC)CC(CC)CO
CHEM : 2,4-Diethyloctane-1-ol
MOL FOR: C12 H26 O1
MOL WT : 186.34
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 19.4285 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 19.5685 E-12 cm3/molecule-sec
HALF-LIFE = 0.547 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 6.559 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

AOP Program (v1.90) Results:
==========
SMILES : CCCC(O)C(CC)CC(CC)CO
CHEM : 2,4-Diethyloctane-1,5-diol
MOL FOR: C12 H26 O2
MOL WT : 202.34
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 28.2880 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 28.5680 E-12 cm3/molecule-sec
HALF-LIFE = 0.374 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 4.493 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

SMILES : CCCCC(CC)CO
CHEM : 2-Ethylhexanol
MOL FOR: C8 H18 O1
MOL WT : 130.23
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 13.0893 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 13.2293 E-12 cm3/molecule-sec
HALF-LIFE = 0.809 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 9.702 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

SMILES : CCC(CO)C(CCC)C(CO)CC
CHEM : 2-Ethyl-3-propyl-4-hydroxymethylhexan-1-ol (C12-diol-2)
MOL FOR: C12 H26 O2
MOL WT : 202.34
--------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 24.2333 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 24.5133 E-12 cm3/molecule-sec
HALF-LIFE = 0.436 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 5.236 Hrs
------- SUMMARY (AOP v1.90): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

CHEM : 2,4,6-Triethyl-3-propylheptane-1,7-diol (C16-diol)
MOL FOR: C15 H32 O2
MOL WT : 244.42
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 28.7487 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.2800 E-12 cm3/molecule-sec

Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 29.0287 E-12 cm3/molecule-sec
HALF-LIFE = 0.368 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 4.422 Hrs
---------- SUMMARY (AOP v1.90): OZONE REACTION ----

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

AOP Program (v1.90) Results:
==========
SMILES : CCCCC(CC)COCCCC
CHEM : 2-Ethylhexyl-n-butyl ether
MOL FOR: C12 H26 O1
MOL WT : 186.34
--------- SUMMARY (AOP v1.90): HYDROXYL RADICALS --------
Hydrogen Abstraction = 35.0835 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 35.0835 E-12 cm3/molecule-sec
HALF-LIFE = 0.305 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 3.658 Hrs

----- SUMMARY (AOP v1.90): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches

Test substance :

Various individal componets of EP-204, CASNO 68609-68-7

Conclusion :

Estimated or experimental rate constants for reaction with hydroxyl radical and predicted half-lives in air are shown in the table. Expected half-lives range from 2.6 hours to 18.6 hours assuming a 12-hhour day and a concentration of 1,500,000 hydroxyl radicals per cubic centimeter.

The material is not considered persistent in the atmosphere.

COMPONENT	SMILES	Rate K*	t1/2(h)
2-Ethylhexanol	CCCCC(CC)CO	13.2	9.7
2-Ethylhexenal	CCCC=C(CC)C=O	50.0	2.6
2-Ethylhexanal	CCCCC(CC)C=O	34.0	3.8
n-Butanol	CCCCO	6.9	18.6
2-Ethyl-1,3-hexanediol	CCCC(O)C(CC)CO	22.2	5.8
2-Ethylhexyl-1,3-dibutyrate	CCCC(OC(=O)CCC)C(CC)COC(=O)CCC	17.5	7.3
n-butyl-n-butyrate	CCCC(=O)OCCCC	10.6	12.1
n-butyraldehyde	CCCC=O	25.4	5.0
2,4-Diethyloctane-1-ol	CCCCC(CC)CC(CC)CO	19.6	6.6
2,4-Diethyloctane-1,5-diol	CCCC(O)C(CC)CC(CC)CO	28.6	4.5
2-Ethyl-3-propyl-4-hydroxy-methylhexan-1-ol (C12)	CCC(CO)C(CCC)C(CO)CC	24.5	5.2
2,4,6-Triethyl-3-propyl-heptane-1,7-diol (C-16)	CC(CO)CC(CC)C(CCC)C(CO)CC	29.3	4.4
2-Ethylhexyl-butyl ether	CCCC(CC)COCCCC	35.1	3.7

* Rate constants in units of x exp12 cm/molec-sec
Half-life in units of hours

Reliability : (2) valid with restrictions

Estimations conducted by an acceptable method are assigned a reliability of 2

Flag : Critical study for SIDS endpoint

10.02.2004 (2)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : > 1 year at 25 °C
t1/2 pH9 : at °C
Deg. product :
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4

Method :

Under aqueous-solution conditions where essentially infinite dilution conditions can be assumed, water stability of the individual components can be estimated based on their chemical properties. Most components of EP-204 have no hydrolysable group and are therefore considered resistant to hydrolysis. These are:

* Aliphatic alcohols
* Aliphatic aldehydes
* Aliphatic carboxylic acids
* Alkenes
* Aliphatic ethers

The following components have hydrolysable groups:

* Aliphatic acetals
* Aliphatic esters

The stability of the aliphatic esters has been estimated using the HYDROWIN Program (v1.67) found in the EPIWIN software (see following

robust summaries).

Stability of acetals cannot be estimated using the EPIWIN software and no definitive information was located on the water stability of these medium to long-chain acetals. As simple acetals are typically resistant to hydrolysis at neutral pH (Vollhardt, K. Peter, Organic Chemistry, WH Freeman and Company, New York 1987, p 640) and as the acetals are a minor component of EP-204, their contribution to the water stability is minimal and they are estimated based on the know chemistry of acetals, to have a a half-life greater than one year.

Test substance :

Various individal componets of EP-204, CASNO 68609-68-7

Conclusion :

EP-204 is considered to be relativley water stable.

Reliability : (2) valid with restrictions

Estimations conducted by an acceptable method as assigned a reliability of 2

Flag : Critical study for SIDS endpoint

27.01.2004 (13)

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : ca. 4.1 year at 25 °C
t1/2 pH9 : ca. 15 day(s) at 25 °C
Deg. product :
Method :
Year :
GLP : no
Test substance : other TS

Method :

Estimation of the hydrolysis of ester components of EP-204 was conducted using the HYDROWIN (ver 1.67) program found in EPIWIN 3.05. The methodology for prediction of hydrolysis rates was developed for the U.S. Environmental Protection Agency and is described in the document: Mill,T., Haag,W., Penwell, P., Pettit, T. and Johnson, H. "Environmental Fate and Exposure Studies Development of a PC-SAR for Hydrolysis: Esters, Alkyl Halides and Epoxides". EPA Contract No. 68-02-4254. Menlo Park, CA: SRI International (1987).

The program calculates the base-catalyzed rate constant for esters using the following equation:

log Kb = 0.92Es{R1} + 0.31Es{R2} + 2.16 sigma*{R1} + 2.30 sigma*{R2} + 2.10 sigmaX{R1} + 1.25 sigmaX{R2} + 2.67

where R1 and R2 designate the carbon shins, Es is the steric factor at the designated position, sigma* is the Taft constant at the designated position, and sigmaX is the Hammett constant at the designated position.

The overall hydrolysis rate constant is equal to the acid-catalyzed plus the base-catalyzed plus the neutral hydrolysis rate constants. In the case of esters it is established that for most esters the base reaction rate dominates by a wide margin and acid and neutral hydrolysis can largely be ignored.

Result :

SMILES : CCCC(=O)OCCCC
CHEM : n-butyl-n-butyrate
MOL FOR: C8 H16 O2
MOL WT : 144.

----- HYDROWIN v1.67 Results ----------

ESTER: R1-C(=O)-O-R2 R1: n-Propyl-

R2: n-Butyl-

Kb hydrolysis at atom # 4: 5.317E-002 L/mol-sec

Total Kb for pH > 8 at 25 C: 5.317E-002 L/mol-sec
Kb Half-Life at pH 8: 150.863 days
Kb Half-Life at pH 7: 4.130 years

Test substance :

n-Butyl-n-butyrate
SMILES: CCCC(=O)OCCCC
Component of EP204

Conclusion :

This material is stable to hydrolysis at pH levels near neutrality having a predicted half-life in the range of 4 years.

Reliability : (2) valid with restrictions

Estimations conducted by an acceptable method as assigned a reliability of 2

Flag : Critical study for SIDS endpoint

01.02.2004 (12)

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : ca. 6.2 year at 25 °C
t1/2 pH9 : ca. 22.6 day(s) at 25 °C
Deg. product :
Method : other (calculated)
Year :
GLP : no
Test substance : other TS

Method :

Estimation of the hydrolysis of ester components of EP-204 was conducted using the HYDROWIN (ver 1.67) program found in EPIWIN 3.05. The methodology for prediction of hydrolysis rates was developed for the U.S. Environmental Protection Agency and is described in the document: Mill,T., Haag,W., Penwell, P., Pettit, T. and Johnson, H. "Environmental Fate and Exposure Studies Development of a PC-SAR for Hydrolysis: Esters, Alkyl Halides and Epoxides". EPA Contract No. 68-02-4254. Menlo Park, CA: SRI International (1987).

The program calculates the base-catalyzed rate constant for esters using the following equation:

log Kb = 0.92Es{R1} + 0.31Es{R2} + 2.16 sigma*{R1} + 2.30 sigma*{R2} + 2.10 sigmaX{R1} + 1.25 sigmaX{R2} + 2.67

where R1 and R2 designate the carbon chains, Es is the steric factor at the

designated position, sigma* is the Taft constant at the designated position, and sigmaX is the Hammett constant at the designated position.

The overall hydrolysis rate constant is equal to the acid-catalyzed plus the base-catalyzed plus the neutral hydrolysis rate constants. In the case of esters it is established that for most esters the base reaction rate dominates by a wide margin and acid and neutral hydrolysis can largely be ignored.

In the case of these n-butyl esters, the Taft and Hammett constants were not available for both positions so the program substituted the values using surrogates.

Result :

SMILES : CCCC(OC(=O)CCC)C(CC)COC(=O)CCC
CHEM : 2-Ethylhexyl-1,3-dibutyrate
MOL FOR: C16 H30 O4
MOL WT : 286.42
---------- HYDROWIN v1.67 Results ----------

NOTE: Fragment(s) on this compound are NOT available from the fragment
library. Substitute(s) have been used!!! Substitute R1, R2, R3, or R4 fragments are marked with double astericks "**".

ESTER: R1-C(=O)-O-R2 R1: n-Propyl-
** R2: -CH(Me)(t-Bu)
Kb hydrolysis at atom # 6: 1.455E-003 L/mol-sec

ESTER: R1-C(=O)-O-R2 R1: n-Propyl-
** R2: iso-Butyl-
Kb hydrolysis at atom # 16: 3.416E-002 L/mol-sec

Total Kb for pH > 8 at 25 deg C : 3.561E-002 L/mol-sec
Kb Half-Life at pH 8: 225.252 days
Kb Half-Life at pH 7: 6.167 years

Test substance :

2-Ethylhexyl-1,3-dibutyrate
SMILES : CCCC(OC(=O)CCC)C(CC)COC(=O)CC
Component of EP-204

Conclusion :

This material is stable to hydrolysis at pH levels near neutrality having a predicted half-life in the range of 6 years

Reliability : (2) valid with restrictions

Estimations conducted by an acceptable method as assigned a reliability of 2

Flag : Critical study for SIDS endpoint
27.01.2004 (3)

3.3.2 DISTRIBUTION

Media : other: Air, water, soil and sediment
Method : Calculation according Mackay, Level III
Year : 2003

Method :

Theoretical Distribution (Fugacity) of EP-204 in the environment was estimated using the MacKay EQC level III model with standard defaults in EPIWIN v 3.05 using equal releases to water, soil and air (EPIWN default) as the means of entry into the environment. The approach used was to take the nine materials represented in the in the preparation at greater than 1% and individually determine their fugacity assuming that one component will not greatly affect the distribution of the other. As the measured vapor pressure of EP-2042 is a function of the partial pressures of each component, it is more appropriate to use the EPIWIN predicted vapor pressure for each component in the calculation. Likewise, individual predicted values for log Kow, Koc, and half-lives were utilized. The biodegradation half-lives that were utilized were EPIWIN generated but were evaluated for consistency with the known biodegradability of the preparation and found to be representative.

Result :

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : 2-Ethylhexenal
  Molecular Wt: 126.2
  Henry's LC  : 0.000488 atm-m3/mole (Henrywin program)
  Vapor Press : 0.463 mm Hg  (Mpbpwin program)
  Log Kow     : 2.62  (Kowwin program)
  Soil Koc    : 171  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.937           4.21         0
   Water     98.4            360          1000
   Soil      0.00879         360          0
   Sediment  0.614           1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       4.01e-012    342         20.7        34.2        2.07
   Water     4.21e-009    419         218         41.9        21.8
   Soil      9.48e-013    0.0374      0           0.00374     0
   Sediment  2.57e-009    0.653       0.0272      0.0653      0.00272

   Persistence Time: 221 hr
   Reaction Time:    291 hr
   Advection Time:   927 hr
   Percent Reacted:  76.1
   Percent Advected: 23.9

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      4.207
      Water:    360
      Soil:     360
      Sediment: 1440
        Biowin estimate: 3.241  (weeks       )
```

```
  Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004


=======================================
  Chem Name   : 2-Ethylhexanal
  Molecular Wt: 128.22
  Henry's LC  : 0.000759 atm-m3/mole (Henry database)
  Vapor Press : 2.18 mm Hg  (Mpbpwin program)
  Log Kow     : 2.71  (Kowwin program)
  Soil Koc    : 210  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       1.81            7.56         0
   Water     97.5            360          1000
   Soil      0.0149          360          0
   Sediment  0.688           1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       7.34e-012    353         38.5        35.3        3.85
   Water     6.14e-009    400         208         40          20.8
   Soil      1.95e-012    0.0612      0           0.00612     0
   Sediment  3.59e-009    0.705       0.0293      0.0705      0.00293

   Persistence Time: 213 hr
   Reaction Time:    282 hr
   Advection Time:   865 hr
   Percent Reacted:  75.4
   Percent Advected: 24.6

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      7.555
      Water:    360
      Soil:     360
      Sediment: 1440
        Biowin estimate: 3.236  (weeks       )

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004

=======================================
  Chem Name   : n-Butanol
  Molecular Wt: 74.12
  Henry's LC  : 8.81e-006 atm-m3/mole (Henry database)
  Vapor Press : 7.78 mm Hg  (Mpbpwin program)
  Log Kow     : 0.88  (Kowwin program)
  Soil Koc    : 3.11  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.255           30           0
   Water     99.6            208          1000
   Soil      0.0177          208          0
   Sediment  0.157           832          0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       1.91e-012    13.4        5.81        1.34        0.581
   Water     1.35e-010    754         226         75.4        22.6
   Soil      7.07e-013    0.134       0           0.0134      0
   Sediment  9.89e-011    0.298       0.00715     0.0298      0.000715
```

```
  Persistence Time: 227 hr
  Reaction Time:    296 hr
  Advection Time:   979 hr
  Percent Reacted:  76.8
  Percent Advected: 23.2

  Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
     Air:      29.95
     Water:    208.1
     Soil:     208.1
     Sediment: 832.3
       Biowin estimate: 3.494  (days-weeks)

  Advection Times (hr):
     Air:      100
     Water:    1000
     Sediment: 5e+004

=====================================
  Chem Name   : 2-Ethyl-1,3-hexanediol
  Molecular Wt: 146.23
  Henry's LC  : 1.37e-008 atm-m3/mole (Henry database)
  Vapor Press : 0.003 mm Hg  (Mpbpwin program)
  Log Kow     : 1.6  (Kowwin program)
  Soil Koc    : 16.3  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
  Air       5.57e-005       11.5         0
  Water     99.8            360          1000
  Soil      0.00397         360          0
  Sediment  0.222           1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
  Air       3.19e-016    0.0114      0.00191     0.00114     0.000191
  Water     1.6e-013     658         342         65.8        34.2
  Soil      1.02e-016    0.0261      0           0.00261     0
  Sediment  1.28e-013    0.366       0.0152      0.0366      0.00152

  Persistence Time: 343 hr
  Reaction Time:    520 hr
  Advection Time:   1e+003 hr
  Percent Reacted:  65.8
  Percent Advected: 34.2

  Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
     Air:      11.55
     Water:    360
     Soil:     360
     Sediment: 1440
       Biowin estimate: 3.196  (weeks       )

  Advection Times (hr):
     Air:      100
     Water:    1000
     Sediment: 5e+004


  Chem Name   : 2-Ethylhexyl-1,3-dibutyrate
  Molecular Wt: 286.42
  Henry's LC  : 3.7e-006 atm-m3/mole (Henrywin program)
  Vapor Press : 0.00147 mm Hg  (Mpbpwin program)
  Log Kow     : 5.17  (Kowwin program)
  Soil Koc    : 6.06e+004  (calc by model)
```

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0322	14.6	0
Water	55.5	360	1000
Soil	0.0115	360	0
Sediment	44.4	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.47e-013	8.17	1.73	0.817	0.173
Water	1.75e-011	573	298	57.3	29.8
Soil	3.03e-017	0.118	0	0.0118	0
Sediment	5.28e-012	115	4.77	11.5	0.477

Persistence Time: 536 hr
Reaction Time: 770 hr
Advection Time: 1.76e+003 hr
Percent Reacted: 69.6
Percent Advected: 30.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 14.64
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 2.847 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Chem Name : n-butyl-n-butyrate
Molecular Wt: 144.22
Henry's LC : 0.000687 atm-m3/mole (Henry database)
Vapor Press : 1.76 mm Hg (Mpbpwin program)
Log Kow : 2.83 (Kowwin program)
Soil Koc : 277 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	4.51	24.2	0
Water	94.9	208	1000
Soil	0.0256	208	0
Sediment	0.561	832	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.3e-011	220	77	22	7.7
Water	3.86e-009	540	162	54	16.2
Soil	1.66e-012	0.146	0	0.0146	0
Sediment	1.49e-009	0.798	0.0192	0.0798	0.00192

Persistence Time: 171 hr
Reaction Time: 224 hr
Advection Time: 714 hr
Percent Reacted: 76.1
Percent Advected: 23.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 24.22
Water: 208.1
Soil: 208.1
Sediment: 832.3
Biowin estimate: 3.319 (days-weeks)

```
 Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004

Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : n-butyraldehyde
  Molecular Wt: 72.11
  Henry's LC  : 0.000115 atm-m3/mole (Henry database)
  Vapor Press : 108 mm Hg  (Mpbpwin program)
  Log Kow     : 0.88  (Kowwin program)
  Soil Koc    : 3.11  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       1.07            10.9         0
   Water     98.7            360          1000
   Soil      0.0105          360          0
   Sediment  0.175           1.44e+003    0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       9.87e-012    185         29.1        18.5        2.91
   Water     2.14e-009    517         269         51.7        26.9
   Soil      6.74e-012    0.055       0           0.0055      0
   Sediment  1.77e-009    0.23        0.00954     0.023       0.000954

   Persistence Time: 272 hr
   Reaction Time:    387 hr
   Advection Time:   914 hr
   Percent Reacted:  70.2
   Percent Advected: 29.8

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      10.92
      Water:    360
      Soil:     360
      Sediment: 1440
        Biowin estimate: 3.062  (weeks       )

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004


Chem Name   : 2-Ethylhexanol
  Molecular Wt: 130.23
  Henry's LC  : 2.65e-005 atm-m3/mole (Henry database)
  Vapor Press : 0.185 mm Hg  (Mpbpwin program)
  Log Kow     : 2.73  (Kowwin program)
  Soil Koc    : 220  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.523           19.4         0
   Water     98.9            208          1000
   Soil      0.0168          208          0
   Sediment  0.519           832          0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       2.17e-012    41.2        11.5        4.12        1.15
   Water     2.22e-010    728         218         72.8        21.8
   Soil      7.5e-014     0.123       0           0.0123      0
   Sediment  9.28e-011    0.954       0.0229      0.0954      0.00229
```

```
 Persistence Time: 221 hr
 Reaction Time:    287 hr
 Advection Time:   960 hr
 Percent Reacted:  77
 Percent Advected: 23

 Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
    Air:      19.4
    Water:    208.1
    Soil:     208.1
    Sediment: 832.3
      Biowin estimate: 3.370  (days-weeks  )

 Advection Times (hr):
    Air:      100
    Water:    1000
    Sediment: 5e+004

Chem Name   : 2,4-Diethyloctane-1-ol
Molecular Wt: 186.34
Henry's LC  : 9.63e-005 atm-m3/mole (Henrywin program)
Vapor Press : 0.00273 mm Hg  (Mpbpwin program)
Log Kow     : 4.62  (Kowwin program)
Soil Koc    : 1.71e+004  (calc by model)

        Concentration   Half-Life    Emissions
          (percent)        (hr)       (kg/hr)
 Air       0.865           13.1         0
 Water     79.6            360          1000
 Soil      0.0233          360          0
 Sediment  19.6            1.44e+003    0

           Fugacity    Reaction    Advection   Reaction    Advection
            (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
 Air       3.82e-012    154         29.1        15.4        2.91
 Water     6.74e-010    516         268         51.6        26.8
 Soil      5.49e-015    0.151       0           0.0151      0
 Sediment  2.07e-010    31.7        1.32        3.17        0.132

 Persistence Time: 337 hr
 Reaction Time:    480 hr
 Advection Time:   1.13e+003 hr
 Percent Reacted:  70.2
 Percent Advected: 29.8

 Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
    Air:      13.12
    Water:    360
    Soil:     360
    Sediment: 1440
      Biowin estimate: 3.246  (weeks       )

 Advection Times (hr):
    Air:      100
    Water:    1000
    Sediment: 5e+004

Chem Name   : 2,4-Diethyloctane-1,5-diol
Molecular Wt: 202.34
Henry's LC  : 2.22e-006 atm-m3/mole (Henrywin program)
Vapor Press : 6.62e-005 mm Hg  (Mpbpwin program)
Liquid VP   : 8.59e-005 mm Hg  (super-cooled)
Melting Pt  : 36.5 deg C (Mpbpwin program)
Log Kow     : 3.49  (Kowwin program)
Soil Koc    : 1.27e+003  (calc by model)
```

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0246	8.99	0
Water	97.6	360	1000
Soil	0.0175	360	0
Sediment	2.35	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.02e-013	6.57	0.852	0.657	0.0852
Water	1.85e-011	650	338	65	33.8
Soil	1.2e-015	0.116	0	0.0116	0
Sediment	7.12e-012	3.92	0.163	0.392	0.0163

Persistence Time: 346 hr
Reaction Time: 524 hr
Advection Time: 1.02e+003 hr
Percent Reacted: 66.1
Percent Advected: 33.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 8.986
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 3.072 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Chem Name : 2-Ethyl-3-propyl-4-hydroxymethylhexan-1-ol (C12-diol-2)
Molecular Wt: 202.34
Henry's LC : 2.22e-006 atm-m3/mole (Henrywin program)
Vapor Press : 4.75e-005 mm Hg (Mpbpwin program)
Liquid VP : 6.26e-005 mm Hg (super-cooled)
Melting Pt : 37.1 deg C (Mpbpwin program)
Log Kow : 3.49 (Kowwin program)
Soil Koc : 1.27e+003 (calc by model)

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.028	10.5	0
Water	97.6	360	1000
Soil	0.0213	360	0
Sediment	2.35	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.15e-013	6.42	0.97	0.642	0.097
Water	1.85e-011	650	338	65	33.8
Soil	1.46e-015	0.142	0	0.0142	0
Sediment	7.12e-012	3.92	0.163	0.392	0.0163

Persistence Time: 346 hr
Reaction Time: 524 hr
Advection Time: 1.02e+003 hr
Percent Reacted: 66.1
Percent Advected: 33.9

```
Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      10.47
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 3.072  (weeks       )

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

```
Chem Name   : 2,4,6-Triethyl-3-propylheptane-1,7-diol (C16-diol)
Molecular Wt: 244.42
Henry's LC  : 5.2e-006 atm-m3/mole (Henrywin program)
Vapor Press : 3.62e-006 mm Hg  (Mpbpwin program)
Liquid VP   : 7.33e-006 mm Hg  (super-cooled)
Melting Pt  : 56 deg C (Mpbpwin program)
Log Kow     : 4.89  (Kowwin program)
Soil Koc    : 3.18e+004  (calc by model)
```

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0371	8.84	0
Water	69.3	360	1000
Soil	0.0652	360	0
Sediment	30.6	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.49e-013	13.1	1.68	1.31	0.168
Water	3.17e-011	602	313	60.2	31.3
Soil	4.55e-016	0.567	0	0.0567	0
Sediment	9.61e-012	66.5	2.77	6.65	0.277

```
Persistence Time: 452 hr
Reaction Time:    662 hr
Advection Time:   1.42e+003 hr
Percent Reacted:  68.3
Percent Advected: 31.7

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      8.844
   Water:    360
   Soil:     360
   Sediment: 1440
     Biowin estimate: 2.979  (weeks)

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

```
Chem Name   : 2-Ethylhexyl-n-butyl ether
Molecular Wt: 186.34
Henry's LC  : 0.0173 atm-m3/mole (Henrywin program)
Vapor Press : 0.262 mm Hg  (Mpbpwin program)
Log Kow     : 4.9  (Kowwin program)
Soil Koc    : 3.26e+004  (calc by model)
```

```
          Concentration   Half-Life    Emissions
            (percent)       (hr)       (kg/hr)
Air         1.73            7.32         0
Water       77.4            208          1000
Soil        0.00918         208          0
Sediment    20.9            832          0

            Fugacity    Reaction    Advection   Reaction    Advection
             (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
Air         4.25e-012    307         32.4        30.7        3.24
Water       6.39e-008    483         145         48.3        14.5
Soil        1.13e-013    0.0573      0           0.00573     0
Sediment    1.16e-008    32.6        0.783       3.26        0.0783

Persistence Time: 187 hr
Reaction Time:    228 hr
Advection Time:   1.05e+003 hr
Percent Reacted:  82.2
Percent Advected: 17.8

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      7.318
   Water:    208.1
   Soil:     208.1
   Sediment: 832.3
     Biowin estimate: 3.375  (days-weeks)

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Test substance :

Various individal componets of EP-204, CASNO 68609-68-7

Conclusion : The components of EP-204 distribute primarily to water. The more volatile components have some distribution to air and 2-ethylhexyl-1,3-dibutyrate, 2,4-Diethyloctane-1-ol and 2,4,6-Triethyl-3-propylheptane-1,7-diol (the C16-diol) have significant distributions in sediment. Soil distribution is not considered important for any component under these conditions of 100% release to water.

COMPONENT	AIR	WATER	SOIL	SEDIMENT
2-Ethylhexanol	0.52	98.9	0.02	0.52
2-Ethylhexenal	0.94	98.4	0.01	0.61
2-Ethylhexanal	1.81	97.5	0.01	0.67
n-Butanol	2.55	99.6	0.02	0.16
2-Ethyl-1,3-hexanediol	<0.1	99.8	0.01	0.22
2-Ethylhexyl-1,3-dibutyrate	0.03	55.5	0.01	44.4
n-Butyl-n-butyrate	4.51	94.9	0.03	0.56
n-Butyraldehyde	1.07	98.7	0.01	0.18
2,4-Diethyloctane-1-ol	0.87	79.6	0.02	19.6
2,4-Diethyloctane-1,5-diol	0.02	97.6	0.02	2.35
2-Ethyl-3-propyl-4-hydroxy methylhexane-1-ol (C12-diol-2)	0.03	98.9	0.02	1.06
2,4,6-Triethyl-3-propyl heptane-1,7-diol (C16-diol)	0.04	69.3	0.06	30.6
2-Ethylhexyl-n-butyl ether	1.74	77.4	0.01	20.9

Reliability : (2) valid with restrictions

Estimations conducted by an acceptable method are assigned a reliability of 2

Flag : Critical study for SIDS endpoint

10.02.2004 (10)

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: Laboratory treatment plant using domestic and synthetic-chemical wastes
Concentration	:	28 mg/l related to Test substance related to
Contact time	:	28 day(s)
Degradation	:	= 60 - 70 (±) % after 28 day(s)
Result	:	
Kinetic of testsubst.	:	5 day(s) = 15 % 10 day(s) = 29 % 17 day(s) = 44 % 24 day(s) = 58 % 28 day(s) = 70 %
Control substance	:	Aniline
Kinetic	:	10 day(s) = 66 % 28 day(s) = 75 %
Method	:	Carbon dioxide evolution test. OECD 301 B (1993) guideline also in accord with ISO 9493:1990
Result	:	See kinetics
Test substance	:	CASNO 68609-68-7 tested as Oxooel 800
Conclusion	:	The test material is biodegradable but does not fully meet the OECD criteria for "readily biodegradable".
Reliability	:	(1) valid without restriction OECD 301 B guideline test under GLP with no deviations.
Flag	:	Critical study for SIDS endpoint

24.12.2004 (5)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : other: calculated from components
Species :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 9.5 calculated

Method :

An estimate of the toxicity of aquatic toxicity of EP-204 was made by using the principle of additivity. If the components are lumped together, assuming no specific joint-toxic action and the same mechanism of action, a rough estimate of the toxicity of EP-204 can be calculated. This is done by summing the individual component's fraction divided by its EC50, dividing this summation by the sum of the fractions (to normalize to 100%) and taking the reciprocal. The EC50 values used are the experimental or estimated single values and the geometric mean if a range of EC50 values found in the literature or estimated from ECOSAR using the seutral organics model

Remark :

Source of LC50 values for fish

2,4-Diethyloctane-1,5-diol: ECOSAR estimate

2-Ethyl-1,3-hexanediol: ECOSAR estimate

2-Ethylhexanol: Value from IUCLID 2000 document for 2-Ethylhexanol (CASNO 104-76-7).

2-Ethylhexenal: Huels AG: Report No. FK 1368, 1997 (unpublished) as cited in IUCLID 2000 document for
2-Ethylhexenal (CASNO 645-62-5).

2-Ethylhexanal: Hoechst AG, unveroeffentlichte Untersuchung 79.0533, (1979) zitiert im Hoechst-GDS vom 29.04.1994 as cited in IUCLID 2000 document for 2-ethylhexanal (CASNO 123-05-7).

n-Butanol: Value from IUCLID 2000 document for n-Butanol (CASNO 71-36-3).

Result :

The calculation for the estimated LC50 for fish is:

Calculation of Estimated LC50 for Fish

Component	[%]	LC50	1/LC50	x[%]
2,4-Diethyloctane-1,5-diol	22.5	6.0	0.166667	3.75
2-Ethyl-1,3-hexanediol	10	257	0.003891	0.038911
2-Ethylhexanol	10	24.4	0.040984	0.409836
2-Ethylhexenal	5	6	0.166667	0.833333
2-Ethylhexanal	5	8	0.125	0.625
n-Butanol	1	1000	0.001	0.001
%Total	[53.5]	Sum of column		5.65808

Sum divided by total [%] 0.105759
1/x = Estimated LC50 9.5 mg/L

Test substance	:	Various individal componets of EP-204, CASNO 68609-68-7
Reliability	:	(2) valid with restrictions Estimations conducted by an acceptable method are assigned a reliability of 2
Flag	:	Critical study for SIDS endpoint

07.11.2004 (11)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC0	:	= 12.5 measured/nominal
EC50	:	= 52 calculated
EC100	:	= 100 measured/nominal
Analytical monitoring	:	yes
Method	:	other: Directive 79/831/EEC, Annex V, Part C, Update of Nov 1989
Year	:	1989
GLP	:	yes
Test substance	:	other TS

Method :

A static toxicity test was conducted using covered 50-ml beakers containing about 20 ml test solution. The dilution water was M4 medium prepared from ultrapure water. The test substance was dissolved in media at a nominal concentration of 100 mg/L by stirring for about 20 hours at 22°. Undissolved test substance was removed by centrifugation for 20 minutes at approximately 17700 G. This stock solution was diluted with test medium to make the final concentrations shown in the table. Groups of 20 daphnids in four replicates of 5 animals were exposed for 48 hours to 6 concentrations of test material and control media. Animals were examined at 0, 3, 6, 24 and 48 hours for signs of toxic effects. Oxygen concentration and pH were measured at 0 and 48 hours using additional replicates. Analytical measurements of test substance concentration was conducted at 0 and 48 hours by extraction of the test media with solvent and capillary GC analysis.

Statistical methods:
The EC50 was assessed using a graphical method on log-probit paper according to Finney Probit Analysis 1971

Result :

Visual inspection of the beakers indicated that some insoluble oily material existed in the test-concentration range.

Concentrations tested and corresponding percent immobilization of Daphnia magna.

CONC mg/L	PERCENT IMMOBILIZATION 24-Hrs	48-Hrs
Control	0	0
3.13	0	0
6.25	0	0
12.5	0	0
25	35	35
50	35	40
100	90	100

Analytical results (concentrations of 3.13, 12.5 and 100 mg/L were measured) showed that the measured concentrations varied from 95.9 - 98.0% of nominal at the start of the study and 95.9 to 105% of nominal at the end (48 hours). From the description of the method, the analysis was conducted by an extraction of the total amount of test medium including any non-dissolved oil that may have been in the test vessel.

Test condition :

Animals were less than 24 hours old at the start of the test and were not fed during the test. During the 48-hour toxicity test, the pH and dissolved oxygen ranged from 7.9 to 8.0 and 7.0 to 8.4 mg/L, respectively. The test temperature was 18-22 °C, the alkalinity was 0.8 to 1.0 mmol/L and hardness 2.2 to 3.1 mmol/L.

Test substance :

CASNO 68609-68-7 tested as Oxo oil 800 (in english report).

Analysis of the test material, based on gc peak areas, was reported as:

2,4-Diethyl-1,5-octanediol	51.9%
2-Ethyl-1,3-hexanediol	9.1%
2-Ethylhexanol	12.6%
Diethyloctanol	5 - 10%
High-boiling components	20%

Conclusion :

Under these conditions, the 48-hour EC50 for Daphnia magna is 52 mg/L and the EC0 is 12.5 mg/L

Reliability : (1) valid without restriction

Guideline study under GLPs with ananlysis of test material and test solutions.

Flag : Critical study for SIDS endpoint

11.02.2004 (8)

Type : other: Calculated from individual components
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : = 12.9 calculated

Method :

An estimate of the toxicity of aquatic toxicity of EP-204 was made by using the principle of additivity. If the components are lumped together, assuming no specific joint-toxic action and the same mechanism of action, a rough estimate of the toxicity of EP-204 can be calculated. This is done by

summing the individual component's fraction divided by its EC50, dividing this summation by the sum of the fractions (to normalize to 100%) and taking the reciprocal. The EC50 values used are the experimental or estimated single values and the geometric mean if a range of EC50 values found in the literature or estimated from ECOSAR using the seutral organics model

Remark :

Source of EC50 values for daphnia

2,4-Diethyloctane-1,5-diol: ECOSAR estimate

2-Ethyl-1,3-hexanediol: ECOSAR estimate

2-Ethylhexanol: Value from IUCLID 2000 document for 2-Ethylhexanol (CASNO 104-76-7).

2-Ethylhexenal: BASF AG, Oekologie-Labor; unveroeffentl. Untersuchung (1165/87) as cited in IUCLID 2000 document for 2-Ethylhexenal (CASNO 645-62-5).

2-Ethylhexanal: BASF AG, Labor Oekologie; unveroeffentlichte Untersuchung, (0423/88) as cited in IUCLID 2000 document for 2-ethylhexanal (CASNO 123-05-7).

n-Butanol: Value from IUCLID 2000 document for n-Butanol (CASNO 71-36-3).

Result :

Calculation of Estimated EC50 for Daphnia

Component	[%]	EC50	1/EC50	x[%]
2,4-Diethyloctane-1,5-diol	22.5	7.1	0.140845	3.169014
2-Ethyl-1,3-hexanediol	10	268	0.003731	0.037313
2-Ethylhexanol	10	39	0.025641	0.25641
2-Ethylhexenal	5	20	0.05	0.25
2-Ethylhexanal	5	11.5	0.086957	0.434783
n-Butanol	1	1000	0.001	0.001
%Total	[53.5]		Sum of column	4.14852

Sum divided by total [%]	0.077542
1/x = Estimated LC50	12.9 mg/L

Test substance :

Various individal componets of EP-204, CASNO 68609-68-7

Reliability : (2) valid with restrictions

Estimations conducted by an acceptable method are assigned a reliability of 2

07.11.2004 (11)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae
Endpoint : other: calculated EC50
Exposure period : 96 hour(s)
Unit : mg/l
EC50 : = 19.3 calculated

Method :

An estimate of the toxicity of aquatic toxicity of EP-204 was made by using the principle of additivity. If the components are lumped together, assuming no specific joint-toxic action and the same mechanism of action, a rough estimate of the toxicity of EP-204 can be calculated. This is done by summing the individual component's fraction divided by its EC50, dividing this summation by the sum of the fractions (to normalize to 100%) and taking the reciprocal. The EC50 values used are the experimental or estimated single values and the geometric mean if a range of EC50 values found in the literature or estimated from ECOSAR using the seutral organics model

Remark :

Source of EC50 values for alga

2,4-Diethyloctane-1,5-diol: ECOSAR estimate

2-Ethyl-1,3-hexanediol: ECOSAR estimate

2-Ethylhexanol: Value from IUCLID 2000 document for 2-Ethylhexanol (CASNO 104-76-7).

2-Ethylhexenal: BASF AG(1988), Labor Oekologie: Unveroeffentlichte Untersuchung: Algentest vom 16.06.1988 (2/x165/87/t72) as cited in IUCLID 2000 document for 2-Ethylhexenal (CASNO 645-62-5).

2-Ethylhexanal: BASF AG, Labor Oekologie; unveroeffentlichte Untersuchung, (0423/88) as cited in IUCLID 2000 document for 2-ethylhexanal (CASNO 123-05-7).

n-Butanol: Value from IUCLID 2000 document for n-Butanol (CASNO 71-36-3).

Result :

Calculation of Estimated EC50 for Green Alga

Component	[%]	EC50	1/EC50	x[%]
2,4-Diethyloctane-1,5-diol	22.5	4.8	0.208333	4.6875
2-Ethyl-1,3-hexanediol	10	164	0.006098	0.060976
2-Ethylhexanol	10	16	0.0625	0.625
2-Ethylhexenal	5	19.3	0.051813	0.259067
2-Ethylhexanal	5	52	0.019231	0.096154
n-Butanol	1	100	0.01	0.01
%Total	[53.5]		Sum of column	5.738697

Sum divided by total [%]	0.107265
1/x = Estimated LC50	19.3 mg/L

Test substance :

Various individal componets of EP-204, CASNO 68609-68-7

Reliability : (2) valid with restrictions

Estimations conducted by an acceptable method are assigned a reliability of 2

Flag : Critical study for SIDS endpoint

07.11.2004 (11)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 5000 mg/kg bw
Species	:	rat
Strain	:	Wistar
Sex	:	male/female
Number of animals	:	10
Vehicle	:	CMC
Doses	:	5000 mg/kg
Method	:	
Year	:	
GLP	:	yes
Test substance	:	

Method :

Groups of five Wistar rates of each sex were dosed by gavage with test material suspended in CMC. Rats had been fasted overnight prior to dosing. Rats were maintained on 12 hour light:dark cycle at 20-24 deg C and 30-70% relative humidity. Rats were observed for 14 days after dosing, sacrificed and macroscopically examined for signs of adverse effects. Animals were weighed as groups on days 3, 7 and 10 of study.

Result :

Mortality;
males 0/5
females 2/5 (day 1 and day 2)

Group bodyweight gain was normal.

Clinical sings included difficulty breathing, loss of equilibrium, piloerection, atony, and general poor condition persisting about 24 hours. Salivation was reported the first 2 to 4 hours after administration.

No chemically related findings were reported at necropsy

Test substance :

CASNO 68609-68-7 tested as Oxoel 800

Conclusion :

The oral LD50 of the test substance is > 5000 mg/kg-bw in male and female Wistar rats.

Reliability : (1) valid without restriction

Guideline like study conducted under GLP

Flag : Critical study for SIDS endpoint

07.11.2004 (14)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	other: Inhalation risk test
Value	:	> .11 mg/l
Species	:	rat
Strain	:	Wistar
Sex	:	male/female
Number of animals	:	

Vehicle	:	
Doses	:	
Exposure time	:	
Method	:	Six Wistar rats of each sex were exposed to a saturated vapor of the test material generated at 20° C for a period of 7 hours.
Result	:	The nominal concentration calculated from the flow rate and material loss was 0.11 mg/L. No animals died during exposure or in the 14-day observation period. No significant clinical signs were observed.
Test substance	:	CASNO 68609-68-7 tested as Oxoel 800
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

07.11.2004 (19)

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-chronic
Species	:	rat
Sex	:	male/female
Strain	:	Fischer 344
Route of admin.	:	gavage
Exposure period	:	13 weeks
Frequency of treatm.	:	5 days/week
Post exposure period	:	none
Doses	:	0, 25, 125, 250 or 500 mg/kg-bw
Control group	:	yes, concurrent vehicle
NOAEL	:	= 125 mg/kg bw
LOAEL	:	= 250 mg/kg bw
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS
Method	:	Animals. F344 rats, 36- to 37-days-old at delivery, were kept singly in stainless steel wire cages. Mean body weight ranges at dosing were (male) 105-114 g and (female) 86-97 g. Animals were acclimated 6 days on a 12-hr photoperiod at 20-24°C and 30-70% relative humidity; food and water were ad lib. In the 13-week study groups of 10 animals of each sex rats received daily oral gavage doses of 0, 25, 125, 250 or 500 mg/kg on 5 consecutive days per week. Doses were prepared daily by dispersing TS in an aqueous solution of Cremophor EL (5 mg/100 ml). Dosing volume was 10 ml/kg, based on weekly body weights. Controls received 5.0 ml/kg vehicle. Concentrations and homogeneity were checked by gas chromatographic

analysis of samples from each dose level at study start and periodically during the 13-week study. Animals were fasted for about16 hr after the last dose and terminated by decapitation under CO2 anesthesia.

In-life observations. Animals were inspected twice daily for morbidity and mortality but only once daily on nontreatment days. Clinical observations were made daily. Body weights were determined on day 01 and weekly thereafter. Animals were palpated on weighing. Average daily food consumption was determined weekly. Blood was collected by retroorbital bleeding from fasted animals on the morning of Days 29 and 84. Standard serum enzyme activities and biochemistry measurements were recorded. Hematology parameters were leucocytes, erythrocytes, hemoglobin, hematocrit, mean corpuscular volume, mean corpuscular hemoglobin, mean corpuscular hemoglobin concentration, platelets, differential leucocytes, and reticulocytes.

Observations at necropsy. Moribund animals were euthanized and dead and euthanized animals were immediately necropsied for gross pathology. At scheduled terminations body and organ weights were measured. At study termination adrenals, brains, kidneys, livers, stomachs, testes, and ovaries from all animals were weighed, and with other organs and tissues listed in U.S. EPA Health Effects Guidelines (1987b) fixed in 4% formalin. All tissues from high dose and control animals were stained with hematoxylin-eosin and examined microscopically. Lungs, livers, spleens, kidneys, stomachs, sternums, femurs, and femur bone marrows were examined microscopically at intermediate dose levels. Skin, eyes, female mammary glands, thigh musculatures, and extraorbital lacrymatory glands were not examined in the absence of signs of toxicity. Livers were also stained with oil red for reticulolipid content and examined microscopically.

Ancillary studies were used only to determine hepatic peroxisome proliferation. Livers were removed at termination and weighed, and cyanide-insensitive pCoA activities and protein concentrations were determined.

Statistical treatment of data. Means and standard deviations were calculated for body weights, food and water consumption, clinical pathology results, and organ weights. Values for test groups were compared with controls in the main study by ANOVA followed by Dunnett's test.

Result :

No rat died on test. There was deacreased weight gain in male and female rats at 500 mg/kg, starting at Week 4 in males and Week 11 in females, amounting to weight losses of 7% in males and 6% in females by Week 13. There were no differences from controls at any treatment level in food consumption.

Clinical pathology. Differences from control values were seen mostly at 84 days. Females at 250 and 500 mg/kg had 30 and 36% decreases in serum ALT activities, respectively. Females at 500 mg/kg had a 16% decrease in serum cholesterol concentration and males at 500 mg/kg had 13% decreases in total protein and albuminconcentrations. There was a 25% increase in reticulocyte numbers in male and female rats at 500 mg/kg.

Necropsy findings: Relative organ weights. Significant differences from controls in rats were moderate and limited to the brain, kidneys, liver, stomach, and testes at 250 and 500 mg/kg (Table 3). Male rat relative brain weights increased by 6% at 500 mg/kg, male kidney weights by 8% at 250

and 16% at 500 mg/kg, male liver weights by 8% at 250 and 29% at 500 mg/kg, male stomach weights by 11% at 500 mg/kg, and testis weights by 5.5% at 500 mg/kg. Female's kidney weights increased by 5% at 250 and 6% at 500 mg/kg, female liver weights by 8% at 250 and 15% at 500 mg/kg, and female stomach weights by 6% at 250 and 16% at 500 mg/kg.

Necropsy findings: Gross observations. Gross lesions differing from controls 500 mg/kg only. 2/10 males and 4/10 females exhibited single or multiple slightly elevated foci in the forestomach. There were no other gross findings.

Necropsy findings: Microscopic findings. Dose-related findings were limited to the forestomach and liver at 500 mg/kg. There was a generalized acannothosis of the forestomach mucosa in 1/10 males with ballooning degeneration of the epithelial wall and acanthosis of the forestomach mucosa in 2/10 males and 5/10 females.There was a moderate decrease in hepatic peripheral lobular fatty infiltration in 4/10 males and 2/10 females and adrenal b-cell hyperplasia in 3/10 females.

Peroxisome proliferation. Hepatic peroxisome proliferation was determined in ancillary 13-week studies by measuring activity of hepatic cyanide-insensitive palmitoyl Coenzyme A in livers at termination. Increases in pCoA activity were 6.5-fold in male rats and 3.4-fold in females at 500 mg/kg, with decreases in body weight gain similar to those in the main study.

Relative Organ Weights at Termination (grams (SD))Weights at other dose levels (25 and 125 mg/kg) did not differ from controls

Males	0	250	500
Brain	0.68 (0.03)	0.70 (0.02)	0.72 (0.02)**
Kidneys	0.69 (0.02)	0.75 (0.02)**	0.81 (0.04)**
Liver	2.77 (0.11)	2.98 (0.08)**	3.57 (0.22)**
Stomach	0.57 (0.03)	0.58 (0.03)	0.63 (0.02)**
Testes	1.11 (0.05)	1.16 (0.07)	1.17 (0.06)*

Females	0	250	500
Brain	1.07 (0.03)	1.1 (0.06)	1.1 (0.04)
Kidneys	0.77 (0.02)	0.81 (0.03)*	0.82 (0.03)**
Liver	2.67 (0.11)	2.88 (0.08)**	3.07 (0.07)**
Stomach	0.71 (0.03)	0.75 (0.03)*	0.82 (0.04)**
Ovaries	0.041(0.003)	0.037(0.005)*	0.039(0.004)

*p 0.05
** p 0.01

Test substance :

2-Ethylhexanol CASNO 104-76-7 (component and surrogate)Purity 99.8% purity by gas chromatography

Conclusion :

The 500-mg/kg dose was associated with significant peroxisome proliferation and systemic toxicity as evidenced by small but statistically significant ($p < 0.01$) reduction in weight gain in rats of each sex. Target organs were the liver and forestomach. The possible testes effects were of special interest and there was a slight increase in relative testis weight at 500 mg/kg but this was not correlated with any morphological changes.

The reduced relative ovarian weight at 250 mg/kg did not occur at 500 mg/kg and is considered incidental. It is concluded that 125 mg/kg was a NOEL based on organ weight changes at 250 mg/kg.

Reliability : (2) valid with restrictions

Published studies are assigned a 2

Flag : Critical study for SIDS endpoint

10.11.2004 (4)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Bacterial reverse mutation assay
System of testing : Salmonella
Test concentration : Varies
Cycotoxic concentr. : See Results
Metabolic activation : with and without
Result : negative
Method : other: National Toxicology Program
Year :
GLP : no data
Test substance : other TS

Method :

As each stain of Salmonella typhimurium is genetically different, using several strains in a test increases the opportunity of detecting a mutagenic chemical. All strains of Salmonella typhimurium used for mutagenicity testing carry a defective (mutant) gene that prevents them from synthesizing the essential amino acid histidine. Mutations leading to the ability to sysntesize histidine are called "back" or "reverse" mutations and the process is referred to as "reversion."

Some test protocols utilize extracts of Aroclor rat or hamster liver enzymes (S9) to promote metabolic conversion of the test chemical. This is necessary since the Salmonella bacterium does not have the mamillian metabolic capabilities.

In the Salmonella assay, a test tube containing a suspension of one strain of Salmonella typhimurium plus S9 mix or plain buffer without S9, is incubated for 20 minutes at 37º C with the test chemical. Control cultures, with all the same ingredients except the test chemical, are also identically incubated. In addition, positive controls with a known potent mutagen, are prepared. After 20 minutes, agar is added to the cultures and the contents of the tubes are thoroughly mixed and poured onto the surface of petri dishes containing standard bacterial culture medium. The plates are incubated, and bacterial colonies that do not require an excess of supplemental histidine appear and grow. These colonies are comprised of Salmonella that have undergone reverse mutation to restore function of the histidine-manufacturing gene. The number of colonies is counted after 2 days.

Several doses (at least 5) of each test chemical and multiple strains of Salmonella typhimurium are used in each experiment. In addition, cultures are set up with and without added S9 liver enzymes at 10% concentration in these studies. ***The pattern and the strength of the mutant response are taken into account in determining the mutagenicity of a chemical. All observed responses are verified in repeat tests. If no increase in mutant

colonies is seen after testing several strains under several different culture conditions, the test chemical is considered to be nonmutagenic in the Salmonella test.

ReferenceMortelmans K, Zeiger E. The Ames Salmonella/microsome mutagenicity assay. Mutat Res. 2000 Nov 20;455(1-2):29-60.

Result :

Summary Information
Study Vehicle: DMSO
Protocol: Preincubation
Result: Negative

Strain: TA100

Dose	No Act (Neg)		No Act (Neg)		10% RLI (Neg)		10% RLI (Neg)		10% HLI (Neg)		10% HLI (Neg)	
ug/Pt.	Mean	sem	Mean	sem	Mean	sem	Mean	sem	Mean	sem	Mean	sem
VC	130	0.3	133	2.9	101	10.7	100	4	124	7.8	124	8.2
3.3	123	1.9	118	9.6	116	39.1	122	3.8	116	16.3	127	42.2
10	137	4.6	111	7.5	119	1	109	10.4	111	9.9	129	43.6
33	134	4.9	115	12.5	115	5.9	116	10.7	117	8.4	99	3.5
100	115	4.5	137	1.8	107	7.2	96	1.7	110	12.4	112	8.8
220			109s	4.9			114	14.5			126	5.4
333	21	0			158	0			180	0		
PC	1133	52	1284	34	800	36	1379	56	973	95.7	1459	98.6

Strain: TA1535

Dose	No Act (Neg)		No Act (Neg)		10% RLI (Neg)		10% RLI (Neg)		10% HLI (Neg)		10% HLI (Neg)	
ug/Pt.	Mn	sem	Mean	sem	Mean	sem	Mean	sem	Mean	sem	Mean	sem
VC	27	3	33	2.3	11	0.7	17	3.8	15	3.2	13	2.7
3.3	27	3.8	33	1	14	1.8	17	1	14	2.1	17	2.6
10	27	3	27	2.7	15	1.8	14	0.3	16	4.1	14	2.6
33	27	1.2	35	0.3	15	1.2	14	1.7	12	3.8	18	0.6
100	22	4.3	31	2.2	12	1.8	13	1.3	13	0.6	14	1
220			25s	2.6			14	0.6			14	2.9
333	T	0			8	0			5s	1.8		
PC	835	13	902	21	66	3.8	91	10.2	84	3.9	90	2.6

Strain: TA1537

Dose	No Act (Neg)		No Act (Neg)		No Act (Neg)		10% RLI (Neg)		10% RLI (Neg)		10% HLI (Neg)		10% HLI (Neg)	
ug/Pt.	Mean	sem	Mean	sem	Mea	sem	Mn	sem	Mn	sem	Mn	sem	Mean	sem
VC	6	0.7	6	0.3	5	0.7	6	1.2	6	0.9	6	1	9	2.6
3.3	8	1.2	4	0.6	6	1.5	5	0.3	7	2.1	5	1.2	9	1.7
10	11	1.9	5	1.2	8	1.9	7	2.5	8	1.5	6	1.5	8	2.2
33	11	2.3	6	0.9	5	0.6	7	1	4	0.7	6	1.2	7	1.5
100	13	2.3	5	1.5	7	2	5	0.7	8	1.8	6	1.2	9	0.9
220					6s	1.7			9	1.2			8	2.6
333	173	0	339	0			12s	2			188s	1		
PC	133	10.7	468	69	370	59	73	4.3	98	11.7	82	7.7	117	38.9

Strain: TA98

Dose	No Act (Neg)		No Act (Neg)		10% RLI (Neg)		10% RLI (Neg)		10% HLI (Neg)		10% HLI (Neg)	
ug/Pt.	Mean	sem	Mn	sem	Mean	sem	Mean	sem	Mean	sem	Mean	sem
VC	17	1.3	18	1.5	20	1.2	20	2.6	28	4.9	33	4.9
3.3	18	1.3	17	2.6	20	3.2	22	1.5	30	0.9	24	4.7
10	12	1.2	15	2.3	23	0.7	23	1.5	24	2	29	0.3
33	16	2	22	1.2	24	4.2	24	3.2	20	2	28	3.2
100	19	1.5	19	0.6	22	2.9	25	1.3	26	1.7	26	1.7
220			18s	1			27	2.1			29	2.6
333	210	0			305	0			9s	3.8		
PC	1049	31	1289	46	544	17	855	31	960	59	820	37.5

Abbreviations:
PC = positive control
VC = vehicle control
RLI = induced male Sprague Dawley rat liver S9
HLI = induced male Syrian hamster liver S9
s = Slight Toxicity; p = Precipitate; x = Slight Toxicity and Precipitate;
T = Toxic; c = Contamination

Test substance :

2-Ethylhexanol CASNO 104-76-7 (component and surrogate)

Conclusion :

Material was non-mutagenic in the presence or absence of standard liver metabolic activating systems

Reliability : (1) valid without restriction

NTP Guideline study with data available for review.

Flag : Critical study for SIDS endpoint

23.12.2004 (7)

Type : Chromosomal aberration test
System of testing : Chinese hamster ovary cells (CHO-W-B1)
Test concentration : See results
Cycotoxic concentr. : See results
Metabolic activation : with and without
Result : negative
Method : other: NTP Protocol
Year :
GLP : no data
Test substance : other TS

Method :

An in vitro assay for chromosomal damage was conducted in cloned Chinese hamster ovary cells (CHO-W-B1) to identify chemicals capable of inducing chromosomal aberrations (CA). The procedure is described in detail by Galloway et al. (1985, 1987). This assay only detects structural chromosomal damage; it does not detect aneuploidy.

Test chemicals were supplied to the testing laboratory as coded aliquots. The substance was tested in cultured CHO cells for induction of SCE and CA, both in the presence and absence of Aroclor 1254-induced male Sprague Dawley rat liver S9 enzymes and cofactor mix. Cultures were handled under gold lights to prevent photolysis of bromodeoxyuridine-substituted DNA. Each test consisted of concurrent solvent and positive controls and of at least three concentrations of test substance; the high dose was limited by toxicity or solubility, or in the absence of either of these

factors, the high dose was limited to 5 mg/mL . A single culture flask per concentration was used. Tests yielding equivocal or positive results generally were repeated.

Cells were harvested in their first mitotic division after the initiation of chemical exposure. Without S9, cells were incubated for 8-12 hours with the test chemical in McCoy's 5A medium supplemented with fetal calf serum, L-glutamine, and antibiotics, then Colcemid was added and incubation was continued for 2 hours. The incubation time and the dose levels selected were determined from the information on cell cycling and toxicity obtained from the prior SCE test; if cell cycle delay was anticipated, the incubation period was extended to permit accumulation of sufficient cells in first metaphase for statistical analysis. The cells were harvested by mitotic shake-off, fixed, and stained with Giemsa. For the CA test with S9, cells were treated with the test chemical and S9 for 2 hrs, after which the treatment medium was removed and the cells incubated for 10 hours in fresh medium, with Colcemid present for the final 2 hrs. Cells were harvested in the same way as for the treatment without S9.

Cells were selected for scoring on the basis of adequate morphology and completeness of karyotype (21 +/- 2 chromosomes). All slides were scored blind and those from a single test were read by the same person. One hundred or two hundred first-division metaphase cells were scored at each dose level. The classes of aberrations that were recorded included "simple" (breaks and terminal deletions), "complex" (rearrangements and translocations), and "other" (pulverized cells, despiralized chromosomes, and cells containing 10 or more aberrations).

Data are presented as the percentage of cells with aberrations. To arrive at a statistical call for a trial, analyses were conducted to assess the presence of a dose-response (trend test) and the significance of the individual dose points compared to the vehicle control (Galloway et al., 1987). For a single trial, a statistically significant ($P<0.05$) difference for one dose point and a significant trend ($P<0.015$) was considered weak evidence for a positive response; significant differences for two or more doses indicated the trial was positive. A strong trend ($P < 0.003$) with a single significant dose level was designated weak positive *, to indicate a high level of induced aberrations. A strongly positive trend ($P < 0.003$), in the absence of a statistically-significant increase at any one dose point, led to an equivocal call. Ultimately, the trial calls were based on a consideration of the statistical analyses as well as the biological information available to the reviewers. Trials that gave a weak positive or positive result were repeated. The overall result for the CA assay was based on an evaluation of the responses in all trials within an activation condition.

Galloway SM, Armstrong MJ, Reuben C. et al. (1987) Chromosome aberrations and sister chromatid exchanges in Chinese hamster ovary cells: Evaluations of 108 chemicals. Environ. Mol. Mutagen. 10(Supplement 10): 1 - 175.

Galloway SM, Bloom AD, Resnick M et al. (1985) Development of a standard protocol for in vitro cytogenetic testing with Chinese hamster ovary cells: Comparison of results for 22 compounds in two laboratories. Environ. Mutagen. 7: 1-51.

Result :

Activation	Trial	Trial Call
No Activation	1	Negative
Induced Rat Liver S9	2	Negative

	Dose µg/mL	Cells	Total Abs. #	Total Abs. Per Cell	Total Abs. % With Abs.	Complex Abs. #	Complex Abs. Per Cell	Complex Abs. % With Abs.	Simple Abs. #	Simple Abs. Per Cell	Simple Abs. % With Abs.	Other Abs. Ab #	Other Abs. % With Abs.
Neg	0	100	0	0	0	0	0	0	0	0	0	0	0
DMSO	0	200	1	0.005	0.5	0	0	0	1	0.01	0.5	0	0
TS	50	200	3	0.015	1	1	0.01	0.5	2	0.01	1	0	0
TS	108	200	1	0.005	0.5	1	0.01	0.5	0	0	0	0	0
TS	233	200	2	0.01	1	0	0	0	2	0.01	1	0	0
TS	500	0	0	0	0	0	0	0	0	0	0	0	0
Mito	0.1	200	40	0.2	16	21	0.11	9	19	0.1	9.5	0	0
	0.4	50	18	0.36	26	11	0.22	18	7	0.14	14	0	0
Trend:			0.366			-0.001			0.2				
Probability:			0.357			0.5			0.421				

	Dose µg/mL	Cells	Total Abs. #	Total Abs. Per Cell	Total Abs. % With Abs.	Complex Abs. #	Complex Abs. Per Cell	Complex Abs. % With Abs.	Simple Abs. #	Simple Abs. Per Cell	Simple Abs. % With Abs.	Other Abs. Ab #	Other Abs. % With Abs.
Neg	0	100	0	0	0	0	0	0	0	0	0	0	0
DMSO	0	200	1	0.005	0.5	0	0	0	1	0.01	0.5	0	0
TS	50	200	0	0	0	0	0	0	0	0	0	0	0
TS	108	200	0	0	0	0	0	0	0	0	0	0	0
TS	233	200	5	0.025	1.5	1	0.01	0.5	4	0.02	1.5	0	0
TS	500	0	0	0	0	0	0	0	0	0	0	0	0
Cyclo	5	200	32	0.16	11.5	12	0.06	5	20	0.1	7.5	0	0
	15	50	11	0.22	20	6	0.12	10	5	0.1	10	0	0
Trend:			1.346			1.343			1.346				
Probability:			0.089			0.09			0.089				

Test substance :

2-Ethylhexanol CASNO 104-76-7 (component and surrogate)Purity 99.8% purity by gas chromatography

Conclusion :

Material did not induce chromosome aberrations in presence or absence of a metabolic activation system

Reliability : (1) valid without restriction

NTP Guideline study with data available for review.

Flag : Critical study for SIDS endpoint

23.12.2004 (7)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	mouse
Sex	:	female
Strain	:	CD-1
Route of admin.	:	oral feed
Exposure period	:	gd 1 to 17
Frequency of treatm.	:	cont
Duration of test	:	
Doses	:	90, 300 or 900 ppm
Control group	:	yes, concurrent vehicle
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS

Method :

Groups of 28 pregnant Swiss (CD-1) mice were treated with 2-ethylhexanol (2EH) in feed at 0, 90, 300 or 900 ppm in feed (corresponding to 0, 0.13, 0.46, 1.49 mmol/kg-day)in a microencapsulated form to prevent reaction with feed and loss of bioavailability. Dosed feed was provided as lib from gestational day 0 to gestational day 17, at which time dams were sacrificed and the products of conception were evaluated. At sacrifice, the number of ovarian corpora lutea and uterine implantation sites, including resorptions, and dead or live fetuses, were recorded. Live and dead fetuses were weighed. Live fetuses were sexed and examined for external, visceral and skeletal malformations and variations using the standard protocols employed by the NTP for developmental toxicity evaluations in mice.

Remark :

Support for a lack of developmental toxicity of 2-ethylhexanol comes from the di-2-ethylhexyl adipate fertility and developmental toxicity study in which a dose of 1080 mg/kg-day to Wistar rats was associated with minimal fetotoxicity and maternal toxicity. [ICI. 1988b. ICI Central Toxicology Laboratory. Di-(2-ethylhexyl)adipate (DEHA): Fertility study in rats. Report CTL/P/2229 (unpublished study). As cited in IRIS, US EPA.]

There is also a dermal developmental toxicity in which groups of 25 pregnant female Fischer 344 rats were treated cutaneously with 2-ethylhexanol at dose levels of 0, 0.3, 1.0, or 3.0 ml/kg/day for 6 hours per day on gestation days 6 through 15. No treatment-related maternal deaths or early pregnancy loss were seen in the treatment groups, but maternal weight gain was significantly reduced during gestation day 6 through 9 in the high-dose animals. Exfoliation and crusting were seen at treatment sites at all dose levels and erythema at dose levels 1.0 and 3.0 ml/kg-day. Low-dose groups, showed an increase in postimplantation loss, decreased litter size, and reduced fetal body weights but this was not observed in the high-dose group. There were no significant increases in incidence of malformations in the 2-ethylhexanol group relative to the sham treatment group. It is concluded that 2-ethylhexanol has no developmental toxicity activity by the dermal route in rats. [Developmental toxicity evaluation of 2-ethylhexanol administered cutaneously to Fischer 344 rats (final report) with attachments and cover letters dated 032189 and 050389, Bushy Run Research Center, EPA/OTS; Doc #86-890000216}

Result :

In the groups treated with 2-ethylhexanol no dams died, delivered early or were removed from study. The pregnancy rate was high (93-96%) and

similar in all groups. In the control group, one litter was fully resorbed. All other pregnant animals had live litters at the gd-17 necropsy. The numbers of live litters evaluated were 27 at 90 and 300 ppm and 26 at 0 and 900 ppm levels. No maternal toxicity observed in this study as a result of 2-ethylhexanol administration. Maternal body weights, absolute weight gains, corrected weight gains, gravid uterine weight absolute liver weight and relative liver weight were similar in all groups. Food consumption was significantly increased on gestational-day 3 in the 900 ppm group but unaffected for all other time points evaluated. The calculated consumption of 2-EH, based on gestational food consumption was 0 (0 mmol/kg), 17 (0.13 mmol/kg), 59 (0.46 mmol/kg) and 191 mg/kg/day (1.49 mmol/kg), for the 0, 90, 300 and 900 ppm groups, respectively.

Exposure to dietary 2-ethylhexanol was not associated with effects on any gestational parameters. The number of corpora lutea, uterine implantation sites (live, dead, resorbed), pre- and postimplantation loss, sex ratio (%, males) and live fetal body weight per litter (all fetuses or separately by sex) were similar across all groups. No treatment-related changes in the incidence of individual, external, visceral, skeletal or total malformations or variations were observed.

In conclusion, there were no maternal or developmental toxic effects of 2-ethylhexanol dietary exposure throughout gestation at any concentration tested with doses ranging as high as 191 mg/kg/day (1.49 mmol/kg).

Test substance :

2-Ethylhexanol CASNO 104-76-7 (component of EP-204)

Reliability : (1) valid without restriction

NTP Guideline study with data available for review.

Flag : Critical study for SIDS endpoint

23.12.2004 (9) (17)

Species	:	rat
Sex	:	female
Strain	:	Crj: CD(SD)
Route of admin.	:	dermal
Exposure period	:	gd 6 to 16, 6 hr per day
Frequency of treatm.	:	daily
Duration of test	:	
Doses	:	1.0, 2.0 or 4.0 mL/kg-day
Control group	:	yes
NOAEL maternal tox.	:	< 1 ml/kg bw
NOAEL teratogen.	:	= 1 ml/kg bw
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS

Method :

Groups of 25 timed-pregnant female CD rats received cutaneous applications of undiluted EHD at dosages of 1.0, 2.0 and 4.0 mL/kg/day for 6 hr/day under occlusion on gestational days 6-15 inclusive. A similar-sized control group received 4.0 mL/kg/day of deionized water with the same exposure regimen.

Result :

Maternal toxicity was present at 4.0 mL/kg-day (reduced body weight gains and mild skin irritation that were not statistically significant, and increased

liver weight that was statistically significant), and also minimally at 1.0 and 2.0 mL/kg-day (mild skin irritation and slightly increased but statistically significant relative liver weight to body weight ratio). At 4.0 mL/kg-day there was one visceral malformation (unilateral hydroureter), increased incidences of three visceral variants (atelectasis, dilated lateral cerebral ventricle, and bilateral dilated ureter), and 13 skeletal variants affecting several skeletal districts. At 2.0 mL/kg-day no malformations were observed, but the incidence of two visceral variants, dilated lateral cerebral ventricle and bilateral dilated ureter, and one skeletal variant, reduced caudal segments, was increased.

Test substance :

2-Ethyl-1,3-hexanediol (CAS No. 94-96-2) (component)

Conclusion :

Under the conditions of this study, the test material was considered to be a weak developmental toxicant at 4.0 and 2.0 mL/kg/day, and 1 mL/kg/day was a "no-observed effect level" for developmental toxicity. As developmenatl toxiciity was oserved only in the presence of maternal toxicity (liver weight increase), the test material is not considered a specific developmental toxin.

Reliability : (1) valid without restriction

Published study, protocol similar to OECD guidelines.

23.12.2004 (16)

(1) BASF, MSDS for Oxoel 800, Ver 2 Druckdatum 27.09.2002

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(3) Estimated usng HYDROWIN 1,67 as found in EPIWIN 3.04 Syracuse Research Cororation and EPA. (April 2000).

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(5) BASF AG, Labor Okologie und Umweltanalytic: unpublished report, Prufung der biologischen Abbaubarkeit von Oxooel 800 in CO2 Entwicklungtest. Project Number 96/0418/22/1 7 Feb 1997.

(6) BASF Technical Data Sheet for EP-204 2-Ethylhexanol Heavies. Product Number 526158, Published December 2003

(7) Data found on NTP public database at http://ntp-apps.niehs.nih.gov/ntp_tox/index.cfm

(8) Determination of the acute effect of Oxo Oil 800 on the swimming ability of the water flea Daphnia magna STRAUS. Final Report Project Number 96/0418/50/2 BASF AG 10.07.1998.

(9) Developmental Toxicity of 2 Ethylhexanol (CAS NO. 104-76-7) in CD-1 Swiss Mice NTP Study: TER90029. Abstract available on the NTP web site and the entire report is available from NTIS.

(10) EQC Level 3 Model as found in EPIWIN v 3.05, Syracuse Research Corporation, Syracuse NY (April 2000).

(11) Estimated by Toxicology and Regulatory Affairs, Freeburg IL 2004

(12) Estimated using HYDROWIN 1,67 as found in EPIWIN 3.05 Syracuse Research Cororation and EPA. (April 2000).

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(20) WSKOW program (v1.40) as found in EPIWIN v 3.05, Syracuse Research Corporation, Syracuse NY (April 2000).